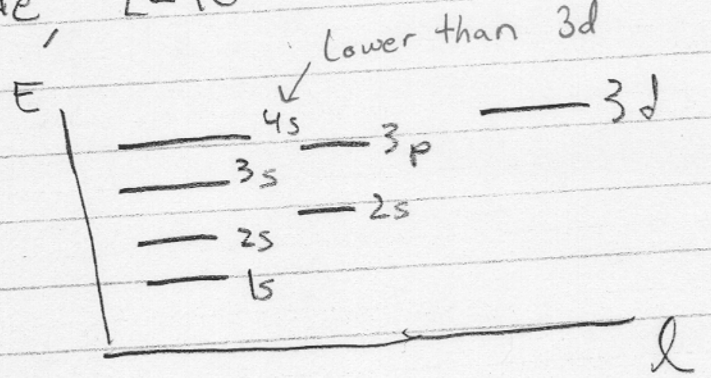
Periodic Table

Ne, $Z=10$



① Ne: $\underbrace{1s^2\,2s^2\,2p^6}_{10}$ it fills the p-shell and is therefore closed

② O: $1s^2\,2s^2\,\underbrace{\uparrow\uparrow\uparrow\downarrow}_{2p^4}$

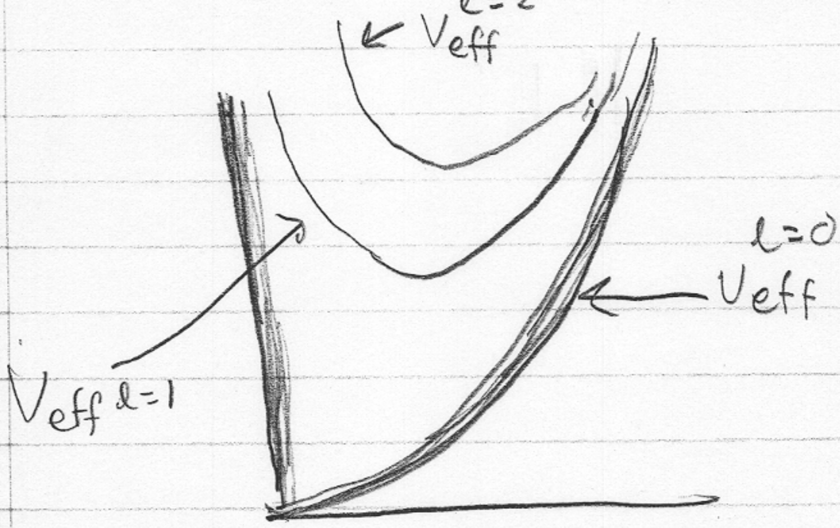
③ $Z=26$ Fe:

$\underbrace{1s^2\,2s^2\,2p^6}_{10}\,\underbrace{3s^2\,3p^6}_{8}\,\underbrace{4s^2}_{2}\,\underbrace{\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow}_{6\text{ electrons}}$

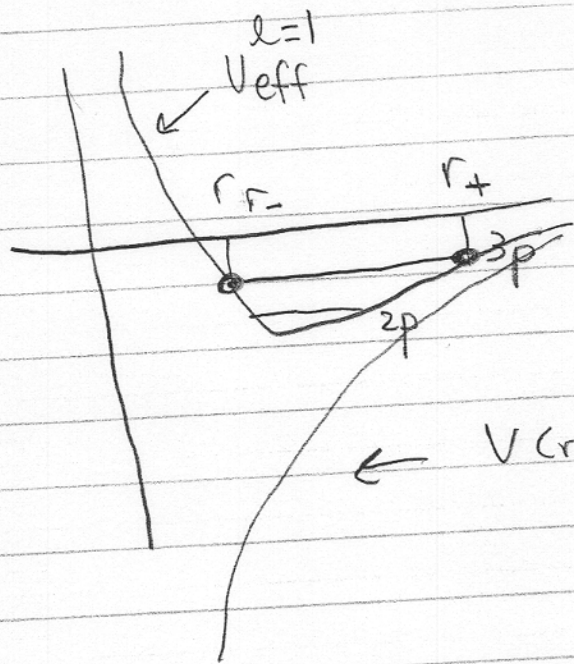
④ Because you are filling up 'd' orbitals $= l=$

$$\underset{\substack{\uparrow\\ \text{Spin}}}{2} \times \underbrace{(2l+1)}_{m=0,\pm1,\pm2} = 2\times 5 = 10$$

② Veff Practise



(3) Inflection Pnts



The radial wave eqn:

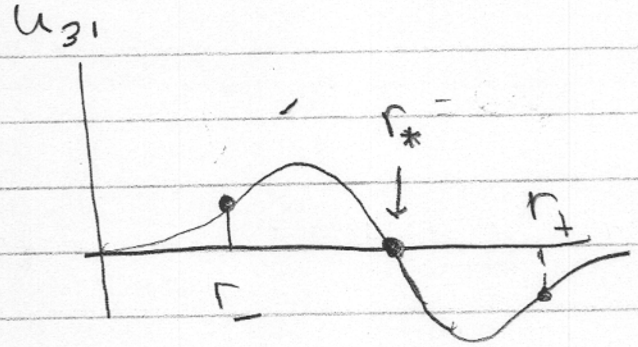
$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + V_{eff}^{\ell=1} u = E u$$

Becomes

$$\frac{d^2u}{dr^2} = -\frac{2m}{\hbar^2}(E - V_{eff})u$$

So infection points happen for $u=0$ and $E-V_{eff}$

The 3p state has $(n-1)-\ell = (3-1)-1=1$ radial excitations and is therefore the first excited state of $V_{eff}^{\ell=1}$



r_-, r_*, r_+ are inflection pnts

$\boxed{r_*}$: Looking at:

$$u_{3p} = u_{31} \propto r R_{31}$$

We see that from table in homework:

$$R_{31} = C(4-\rho)\rho e^{-\rho/2} \quad \text{with} \quad \rho = \frac{2r}{3a_0}$$

is zero at:

$$\rho_* = 4 \quad \text{or} \quad \frac{2r_*}{3a_0} = 4 \Rightarrow \boxed{r_* = 6a_0}$$

$\boxed{r_\pm}$ To find $r_\pm$ we set

$$E = V_{eff}^{\ell=1}(r) \qquad \ell(\ell+1)=2$$

$$\underbrace{-\frac{\hbar^2}{2ma_0^2}\frac{1}{3^2}}_{= -\frac{13.6\,eV}{3^2}} = -\frac{e^2}{4\pi\varepsilon_0 r} + \frac{2\hbar^2}{2mr^2}$$

Lets measure with, $\bar{r} = r/a_0$.

$$-\frac{\hbar^2}{2ma_0^2}\frac{1}{3^2} = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{a_0}\frac{1}{\bar{r}} + \frac{2\hbar^2}{2ma_0^2}\frac{1}{\bar{r}^2}$$

Now recalling: (Bohr Model)

$$\frac{e^2}{4\pi\varepsilon_0 a_0} = 2\frac{\hbar^2}{2ma_0^2} = 27.2\ eV$$

We find

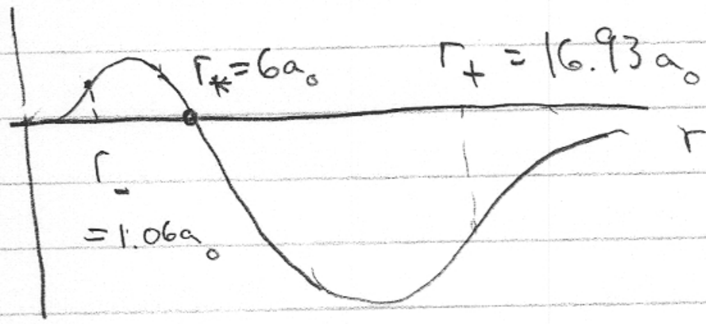
$$-\frac{1}{3^2} = -\frac{2}{\bar{r}} + \frac{2}{\bar{r}^2}$$

So

$$-\frac{\bar{r}^2}{9} = -2\bar{r} + 2 \Rightarrow -\frac{1}{9}\bar{r}^2 + 2\bar{r} - 2 = 0$$

$$\bar{r}_{\pm} = 3(3 \pm \sqrt{7})\, a_0$$

$$\bar{r}_{+} = 16.93\, a_0 \qquad \bar{r}_{-} = 1.062\, a_0$$



Quad eqn

$$+\bar{r}^2 - 18\bar{r} + 18 = 0$$

$$\bar{r} = 9 \pm \sqrt{9^2 - 18}$$

$$\bar{r} = 9 \pm \sqrt{9}\sqrt{9-2}$$

$$\bar{r} = 9 \pm 3\sqrt{7}$$

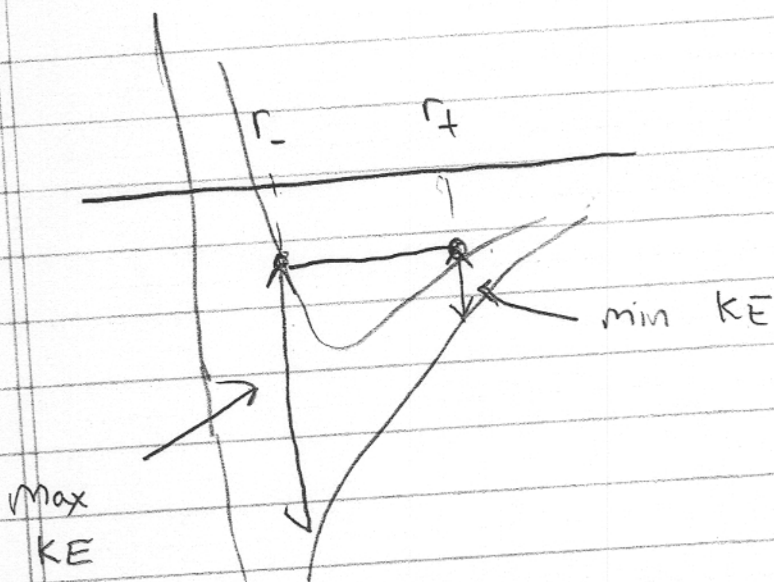
$$r = 9 \pm 3\sqrt{7}\, a_0$$

$$r = 3(3 \pm \sqrt{7})\, a_0$$

Classical orbits

Using E-consv!

$$E = V(r) + KE$$



Using the results of previous section

$r_- = 1.062 a_0$ while $r_+ = 16.93 a_0$

minimum rad   maximum rad

$$KE_{max} = E - V(r_{min})$$

$$= \left(\frac{-\hbar^2}{2 m a_0^2} \frac{1}{3^2}\right) - \frac{e^2}{4\pi\varepsilon_0 a_0} \frac{1}{1.062}$$

using

$$\frac{\hbar^2}{2ma_0^2} = 13.6\,eV \qquad \frac{e^2}{4\pi\varepsilon_0 a_0} = 27.2\,eV$$

$$KE = -13.6\,eV\left(\frac{1}{9} - \frac{2}{1.062}\right)$$

$$KE_{max} = \underbrace{\frac{\hbar^2}{2ma_0^2}}_{13.6eV}(1.77) = \frac{1}{2}mv_{max}^2$$

So :

Too fancy (but cooler!)

$$\underbrace{\frac{1}{2}mc^2\alpha^2}_{13.6eV}\left(\frac{v_{max}}{c\,\alpha}\right)^2 = \underbrace{\frac{\hbar^2}{2ma_0^2}}_{13.6eV}\,1.77$$

$$v_{max} = \sqrt{1.77}\;c\,\alpha$$

← simple way

$$\frac{v_{max}}{c} = 1.33\,\alpha = 0.0097$$

$$v_{max} = \sqrt{\frac{2K_{max}}{m}}$$

$$v_{max} = \sqrt{\frac{2(13.6eV)(1.77)}{(511000\,eV)}}\;c = 0.0097\,c$$

$$K_{min} = E - V(r_{max})$$

$$= \left(-\frac{\hbar^2}{2ma_0^2} \frac{1}{3^2} \right) - \frac{e^2}{4\pi\varepsilon_0 a_0} \frac{1}{16.93}$$

$$K_{min} = -13.6 \left(\frac{1}{9} - \frac{2}{16.93} \right)$$

$$K_{min} = +13.6\,eV\,(0.0070)$$

Now

$$\frac{1}{2} m \cdot v_{min}^2 = K_{min}$$

$$v_{min} = \sqrt{\frac{2K_{min}}{m}}$$

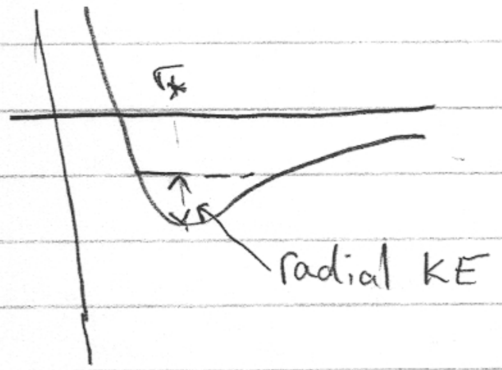
$$v_{min} = c \left(\frac{2K_{min}}{mc^2} \right)^{1/2}$$

$$\frac{v_{min}}{c} = \sqrt{\frac{2\,(13.6\,eV)(0.007)}{511000\,eV}} = 6 \times 10^{-4}$$

$$\frac{v_{max}}{v_{min}} \simeq 16$$

The max radial ~~speed~~ velocity

$$\frac{1}{2} m v_r^2 = E - V_{eff}(r)$$



See Homework #10 where we found the min. of V_{eff}

From homework: $r_* = \underbrace{l(l+1)}\, a_0$

$2 = l(l+1)$ since $l =$ for p states

$$K_r = -\frac{\hbar^2}{2ma_0^2}\frac{1}{3^2} - \left(\frac{-e^2}{4\pi\varepsilon_0 r} + \frac{2\hbar^2}{2mr^2}\right)$$

radial KE

Substituting, $r^* = 2a_0$:

$$K_r = -\frac{\hbar^2}{2ma_0^2}\frac{1}{9} + \frac{e^2}{4\pi\varepsilon_0}\frac{1}{a_0 \cdot 2} - \frac{2\hbar^2}{2ma_0^2 \cdot 4}\Big)$$

Using

$$\frac{\hbar^2}{2ma_0^2} = \frac{e^2}{4\pi\varepsilon_0 a_0}\frac{1}{2} = 13.6\,eV$$

We have

$$K_r = 13.6\,\text{eV}\left(-\frac{1}{9} + 1 \quad -\frac{2}{4}\right)$$

$$K_r = 13.6\,\text{eV}\ (0.389)$$

So:

$$v_r^{max} = \sqrt{\frac{2K_r}{m}} = c\sqrt{\frac{2K_r}{mc^2}}$$

$$\frac{v_r^{max}}{c} = \left(\frac{2\cdot(13.6\,\text{eV})(0.389)}{511{,}000}\right)^{1/2}$$

$$\frac{v_r^{max}}{c} = 0.0045$$

$$\frac{V^{max}}{V^{max}_{radial}} = 2.131$$

Average PE, KE, Ang KE

$$\overline{PE} = \int_0^\infty |4\pi r^2 R_{21}| \cdot V(r)\, dr$$

$$V(r) = \frac{-e^2}{4\pi\varepsilon_0 r}$$

$$R_{21} = \frac{1}{\sqrt{96\pi a_0^3}} \left(\frac{r}{a_0}\right) e^{-r/2a_0}$$

$$4\pi r^2 R^2 = \frac{4\pi r^2}{96\pi a_0^3} \left(\frac{r}{a_0}\right)^2 e^{-r/a_0}$$

$$\overline{PE} = \int_0^\infty dr \frac{4\pi}{96\pi\ a_0^3} r^2 \left(\frac{r}{a_0}\right)^2 e^{-r/a_0} \frac{-e^2}{4\pi\varepsilon_0} \frac{1}{r}$$

$$= \frac{4\pi}{96\pi} \int_0^\infty \frac{dr}{a_0} \frac{r^2}{a_0^2} \left(\frac{r}{a_0}\right)^2 e^{-r/a_0} \left(\frac{-e^2}{4\pi\varepsilon_0 a_0}\right)\left(\frac{a_0}{r}\right)$$

$$= \frac{4\pi}{96\pi} \overbrace{\left(\frac{-e^2}{4\pi\varepsilon_0 a_0}\right)}^{= -27.2\text{eV}} \int_0^\infty dy\, y^4 e^{-y} \frac{1}{y} \qquad y = \frac{r}{a_0}$$

$$PE = \frac{4\cancel{\pi}}{96\cancel{\pi}} \overbrace{\left(\frac{-e^2}{4\pi\varepsilon_0 a_0}\right)}^{-27.2\,eV} \underbrace{\int_0^\infty dy\, y^3 e^{-y}}_{=3!}$$

$$\boxed{\overline{PE} = -(27.2\,eV)\ \frac{1}{4}}$$

$$\overline{Ang\,KE} = \int_0^\infty dr\, 4\pi r^2 R_{21} \quad \frac{\overset{\overset{l=1}{\downarrow}}{l}(l+1)\hbar^2}{2mr^2}$$

$$\overline{AKE} = \int_0^\infty dr \frac{4\pi}{96\pi a_0^3} r^2 \left(\frac{r}{a_0}\right)^2 e^{-r/a_0} \quad \frac{2\hbar^2}{2m}$$

$$= \frac{4\pi}{96\pi} \int_0^\infty \frac{dr}{a_0} \left(\frac{r}{a_0}\right)^4 e^{-r/a_0} \frac{2\hbar^2}{2ma_0^2} \left(\frac{a_0}{r}\right)^2$$

$$\overline{AKE} = \frac{4\pi\, 2}{96\pi} \underbrace{\left(\frac{\hbar^2}{2ma_0^2}\right)}_{=13.6\,eV} \underbrace{\int_0^\infty dy\, y^4 e^{-y} \frac{1}{y^2}}_{=2!}$$

Note $\leftarrow$ remember Bohr

$$\frac{\hbar^2}{2ma_0^2} = \frac{e^2}{4\pi\varepsilon_0 a_0}\left(\frac{1}{2}\right)$$

$$= 13.6\,eV$$

$$\boxed{\overline{AKE} = 13.6\,eV \left(\frac{1}{6}\right)}$$

Then

$$\overline{KE} = \overline{E} - \overline{V}$$

$$= \frac{-13.6\,eV}{4} - \frac{-27.2\,eV}{4}$$

$$\overline{KE} = \frac{+13.6\,eV}{4}$$

Now the Challenge - Skipped if pressed for time

$$\overline{KE} = \overline{\text{Radial KE}} + \overline{\text{Angular KE}}$$

Skip if pressed for time! Just Look jump to Eq ** on next page

$$\text{Radiall KE} = \int_0^\infty dr \left(u^* \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial r^2} \right] u \right)$$

With alegebra, using $\frac{\partial}{\partial r} = \frac{1}{a_0} \frac{\partial}{\partial y}$:

$$u^* \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial r^2} u = \frac{\hbar^2}{2ma_0^2} u \left(-\frac{d^2}{dy^2} u \right)$$

wher

$$u = \sqrt{\frac{4\pi}{96\pi a_0^3}}\, a_0 \left(y^2 e^{-y/2} \right) \quad \text{where } y = \frac{r}{a_0}$$

So we find :

$$u^* \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial r^2} u = \left(\frac{\hbar^2}{2ma_0^2} \right) \left(\frac{4\pi}{96\pi a_0^3} \right) a_0^2 \left[y^2 e^{-y/2} \frac{-d^2}{dy^2} y^2 e^{-y/2} \right]$$

$$= \left(\frac{\hbar^2}{2ma_0^2} \right) \left(\frac{4\pi}{96\pi a_0^3} \right) a_0^2 \left[\frac{-1}{4} e^{-y} y^2 (8 - 8y + y^2) \right]$$

So

We have

$$\overline{\text{Radial KE}} = \int_0^\infty dr \left(\frac{\hbar^2}{2ma_0^2}\right)\left(\frac{4\pi}{96\pi a_0^3}\right) a_0$$

$$\times \left[\frac{-1}{4} e^{-y}\left(y^4 - 8y^3 + 8y^2\right)\right]$$

$$= \left(\frac{\hbar^2}{2ma_0^2}\right) \frac{4\pi}{96\pi} \left(\frac{-1}{4}\right) \int_0^\infty dy\, e^{-y} \left(y^4 - 8y^3 + 8y^2\right)$$

$$= \frac{\hbar^2}{2ma_0^2}\left(\frac{4\pi}{96\pi}\right)\left(\frac{-1}{4}\right)\left[4! - 8\cdot 3! + 8\cdot 2!\right]$$

(***) $\overline{\text{Radial KE}} = 13.6\text{eV} \cdot \frac{1}{12}$

Note then:

$$\overline{KE} = \overline{\text{Radial KE}} + \overline{AKE}$$

$$= 13.6\text{eV}\left(\frac{1}{12} + \frac{1}{6}\right) = +\frac{13.6}{4}$$

So

$$\overline{E} = \frac{-13.6\text{eV}}{4} \stackrel{?}{=} \left(\overline{PE} + \overline{KE}\right) = -\frac{27.2\text{eV}}{4} + \frac{13.6\text{eV}}{4}$$

$$-13.6/4 \stackrel{\checkmark}{=} -13.6/4$$